INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XXXIX, 873–875 (1991)

Subject Index to Volume XXXIX

Ab initio, 31, 71, 123, 269, 411, 449, 541, 625, 767, 839
Ab initio Hartree–Fock band structure calculation, 149
Alkali cations, 131
Anisotropic spectral moments, 755
Anomeric effect, 851
Approximate density matrices, 823
Ar core, 197
Aromaticity, 605
Atom–atom scattering, 159
Atomic nucleus, 805, 813
Atoms, 615
Azabenzene, 309
Azaborine formation, 787

B functions, 625
Basis functions, 625
Basis set, 163, 411, 449
Basis-set expansion method, 813
Benzene, 309
Bifurcated water dimer, 449
Body-fixed axis system, 183
Bonding, 689
Borazine derivatives, 787
Born–Oppenheimer Principle, 437
Broad-band emission, 287
Buckminsterfullerene (BF), 331

C_6 coefficients, 667
Cage structures, 331
Cartesian force constant redundancy, 19
Cellular multiple-scattering-$X_{\alpha\beta}$ calculation, 689
Channel-three decay, 309
Charge-transfer (CT) intensity, 299
Chemisorption, 839
Closed-shell molecules, 487
Clusters, 699
Coherence, 353
Coherent multiphoton excitation, 387
Collision-induced emission, 287
Configuration interaction (CI) calculations, 649
Conformation, 851
Core electrons, 747
Core hole spectra, 455
Coriolis coupling constant, 423
Correlation energy, 649
Crystalline environment, 541
Curve crossing, 523
Cyclotrimers, 787

Dense gases, 399
Density functional theory, 585
Diatomic molecules, 523
Dinaphthonorbornadiene (DNND), 345
Dipolar oscillator strength distribution, 755
Dipole moments, 269
Dirac–Fock (DF) self-consistent field (SCF) method, 487
DNA strand breaks, 709
Dry electron, 47
Dynamic dipole polarizabilities, 667

Effective core potentials (ECP) calculations, 197
Eigenfunctions, 173, 649
Eigenvalues, 59, 173
Electron hydration process, 47
Electronic absorption spectra, 211
Electronic excited states, 681
Electronic structure characteristics, of saturated molecules, 11
Embedding, 839
Energy deposition mechanisms, 709
Enzymes, 767
Exchange energy, 823
Exchange energy density ε_x, 585
Excitable biomembranes, 131
Exciton interactions, 345
Exciton model, 345

Finite nuclear size, 487
Finite-size effect (FSE), 805
Floating spherical Gaussian orbital (FSGO) model, 115

Gas phase, 287
Gaussian functions, 163
Gaussian integral, 123
Gaussian-type basis functions, 487
Generator coordinate approximation (GCA), 523
Green matrix, 839
Ground state, 615

© 1991 John Wiley & Sons, Inc.

Hamiltonian, 183, 523
Hamiltonian method, 11
Harmonic force constant matrix (FCM), 19
Harmonic oscillator interaction, 173
Hartree–Fock, 411, 681
Hartree-Fock theory, 585
Hess–Schaad analysis, 605
HF-SCF-band structures, 839
Husimi function, 823
Hydrogen bonding, 449
Hyperradius, 657

INDO/CI spectroscopic model, 331
INDO/S-CI procedure, 211
Infrared absorption, 437
Intermediate neglect of differential overlap (INDO) model, 31
Isotropic spectral moments, 755

Kasha, Michael, 235
Kekulé structures, 605
Kinetic energy, 615
Kinetic energy density t, 585

Lattice energy, 149
LCAO method, 729
Lewis–Langmuir model, 657
Liouville equation, 353
Liver alcohol dehydrogenase (LADH) catalytic mechanism, 767

Many-body theory, 173, 455
Many-electron atom, 657
Maximum overlap, 729
Meller–Plesset theory, 131
Metal azides, 149
Modified neglect of diatomic overlap (MNDO) calculations, 787
Modified virtual orbitals (MVO), 649
Molecular core electron spectroscopies, 455
Molecular orbital (MO) calculations, 211
Molecular orbital theory, 455
Molecular point symmetry group, 729
Molecules, 11, 371, 541, 605
Monohydrates, 131
Monte-Carlo scheme, 709
Mulliken charge-transfer (CT) model, 299
Multilevel systems, 387
Multiple scattering X-alpha (MS-X_α) calculation method, 71
Multireference double excitation-configuration interaction (MRD-CI) calculations, 541

Net sign analysis, 59
Nonadiabatic solvation, 561
Non-muffin tin (NMT) correction, 71
Nonrelativistic atoms, 805, 813
Nuclear magnetic resonance (NMR) spectra, 371

One-body virial, 615
One-dimensional simple quantal systems, 59
Optimal control theory, 325
Optimal pulse, 325
Organometallic systems, 115
Orthogonalization procedure, 747
Orthogonal subspaces, 747

Pauli potential, 615
Perturbation theory, 561
Point-change (PC) model, 813
Point group symmetry, 19
Polyatomic molecules, 387
Population, 353
Pseudopotential, 115
P states, 805

Quantum chemistry, current problems in, 3
Quasi-degenerate many-body perturbation theory (QDMBPT), 269

Radiation, 709
Radiationless decay, 309
Rainbow angle, 159
Raman intensities, 411
Random phase approximation, 755
Rate constant, 561
Reduced class coefficients (RCCS), 593
Relativistic atoms, 805, 813
Rotational bands, 423
Rovibrational transitions, 423
RRKM theory, 561
Rydberg spectra, 399

SCF calculations, 163
SCF MO methods, 767
Schrödinger equation, 657
Second-order polarization propagator approximation (SOPPA), 371, 667
Second-row transition metal species, 31
Self-consistent modified extended Huckel (SC-MEH-MO) calculations, 699
Single-cycle class, 593
Single-excitations-adapted molecular orbitals (SEAMOS), 681

Singlet oxygen, 251
Solvation free energy, 851
Solvent, 851
Stimulated emission pumping (SEP), 325
STO-2G method, 123
S-type Gaussian functions, 163
Subexcitation electron, energy degradation, 47
Superconductors, 699
Symmetric group, 593
Symmetry-adapted cluster configuration interaction (SAC-CI) theory, 93
Symmetry-adapted cluster (SAC) theory, 93
Symmetry orbitals, 729

Three-center nuclear attraction integrals, 625
Transferability, 11
Transition-metal compounds, 299
Transition-metal molecules, 689
Transition metals, 197
Transition moments, 269
Triatomic system, 183
Two-dimensional simple quantal systems, 59

Ultrafast time-resolved absorption spectroscopy, 353
Uniformly charged sphere (UCS) model, 813

Valence orbitals, 747
van der Waals interaction, on infrared intensities, 437
Vibration-rotation coordinates, 183

White blood cell phagocytosis, 251
Wigner function, 823

A

Å
I

A

A

A
A
A

B
C
B
B
B
B

B

B

C
C
C

©

INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY, VOL. XXXIX, 883–886 (1991)

Author Index to Volume XXXIX

Abu-Eittah, R.
—; Hamed, M. M.; Mohamed, A. A.: A Study on the Electronic Spectra of Vinylpyridines and 1,2-(Dipyridyl)Ethylenes. Molecular Orbital Calculations, 211
Ågren, H.
Interaction Between Theory and Experiment in Molecular Core Electron Spectroscopies, 455
Amirav, A.
—; Even, U.; Jortner, J.: The Dynamics of Equally Spaced Multilevel Model Systems, 387
Anderson, W. P.
—; Cundari, T. R.; Zerner, M. C.: An Intermediate Neglect of Differential Overlap Model for Second-Row Transition Metal Species, 31
Andres, J. See Tapia, O., 767
Asaf, U. See McGlynn, S. P., 399
Avery, J.
—; Goodson, D. Z.; Herschbach, D. R.: Approximate Separation of the Hyperradius in the Many-Particle Schrödinger Equation, 657

Banerjee, A.
Construction of Orthogonal Subspaces, 747
Bassez-Muguet, M.-P. See Muguet, F. F., 449
Baxter, E. See Boudreaux, E. A., 699
Bosanac, S. D. See Murrell, J. N., 159
Boudreaux, E. A.
—; Baxter, E.: SC-MEH-MO Calculations on High T_c Superconductors. 1: The $YBa_2Cu_8O_{26}^+$ Cluster in $YBa_2Cu_3O_7$*, 699
Broeckhove, J.
—; Lathouwers, L.: A Realistic Model for Curve Crossing in Diatomic Molecules, 523
Buenker, R. S. See Chapman, D. A., 541

Campillo, M. See Tapia, O., 767
Cardenas, R. See Tapia, O., 767
Castro, M.
—; Keller, J.; Mareca, P.: Bonding in Heteronuclear Transition-Metal Diatomics: NbIr, 689

Chang, W. L. See Yeh, C. Y., 353
Chapman, D. A.
—; Roszak, S.; Keegstra, P. B.; Hariharan, P. C.; Kaufman, J. J.; Buenker, R. S., 541
Chatterjee, A.
—; Holley, W. R.: Energy Deposition Mechanisms and Biochemical Aspects of DNA Strand Breaks by Ionizing Radiation, 709
Cioslowski, J.
Single-Excitations-Adapted Molecular Orbitals for a Simplified Description of Electronic Excited States, 681
Clementi, E. See Mohanty, A., 487
Colonna-Cesari, F. See Tapia, O., 767
Colson, S. D. See Thiel, Y., 423
Connolly, J. S. See Strickler, S. J., 345
Cormier, R. A. See Strickler, S. J., 345
Crosby, G. A. See Parker, W. L., 299
Cundari, T. R. See Anderson, W. P., 31

Diercksen, G. H. F.
—; Oddershede, J.; Paidarova, I.; Sabin, J. R.: A Calculation of the Isotropic and Anisotropic Spectral Moments of the Dipole Oscillator Strength Distribution of N_2, 755
—; See Sauer, S. P. A., 667

Eriksson, L. A. See Murrell, J. N., 159
Even, U. See Amirav, A., 387

Felps, S. See McGlynn, S. P., 399
Feng, J.
—; Li, J.; Li, Z.; Zerner, M. C.: Quantum Chemical Calculations on Buckminsterfullerene and Related Structures. II. The Electronic Structure and Spectra of Some C_n and C_nCa^{2+} Cages, 331
Fink, E. H.
—; Setzer, K. D.; Wildt, J.; Ramsay, D. A.; Vervloet, M.: Collision-induced Emission of $O_2(b^1\Sigma_g^+ \rightarrow a^1\Delta_g)$ in the Gas Phase, 287
Fleck, O.
—; Ladik, J.: Theoretical Treatment of Chemisorption Using an Ab Initio SCF Green-Matrix Formalism, 839

© 1991 John Wiley & Sons, Inc.

Freed, K. F. See Kanzler, A.W., 269
Fueno, H. See Tachibana, A., 561
Fujimura, N. See Hasegawa, T., 805
—; See Matsuoka, O., 813

Gineitytė, V.
—; Shatkovskaya, D.: Transferability of the Electronic Structure Characteristics of Saturated Molecules, 11
Goodman, L. See Ozkabak, A. G., 411
Goodson, D. Z. See Avery, J., 657
Green, A. See Mann, A., 47

Hall, G. G.
Aromaticity Measured by Kekulé Structures, 605
Hamed, M. M. See Abu-Eittah, R., 211
Hariharan, P. C. See Chapman, D. A., 541
Hasegawa, T.
—; Fujimura, N.; Matsuoka, O.: Hydrogenlike Atoms in Uniformly Charged Sphere Model of Atomic Nucleus. I. Reference Calculations of Energy Levels, 805
—; See Matsuoka, O., 813
Herschbach, D. R. See Avery, J., 657
Holley, W. R. See Chatterjee, A., 709
Homeier, H. H. H.
—; Steinborn, E. O.: Improved Quadrature Methods for Three-Center Nuclear Attraction Integrals with Exponential-Type Basis Functions, 625
Howard, S. T.
—; Huke, J. P.; Parsons, I. W.; Till, S. J.: Transition Properties from Multiple Scattering X-Alpha Calculations: A Study of NO_2, 71
Huke, J. P. See Howard, S. T., 71

Jensen, J. O.
—; Leonard, J. M.: Calculations Using a Set of Evenly Spaced *S*-type Gaussian Functions, 163
Jiancheng, X.
—; Shouping, J.: The Rapid Estimate of a Gauss Integral, 123
Jortner, J. See Amirav, A., 387

Kanzler, A. W.
—; Sun, H.; Freed, K. F.: Dipole Moments, Transition Moments, Oscillator Strengths, Radiative Lifetimes, and Overtone Intensities for CH and CH^+ as Computed by Quasi-degenerate Many-Body Perturbation Theory, 269
Kariev, A. M.
—; Ovchinnikov, A. A.: Monohydration Selectivity Mechanism of Alkali Cations in the Potassium Channel of Excitable Biomembranes, 131
Katriel, J.
A Partial Recurrence Relation for Reduced Class Coefficients of the Symmetric Group, 593
Kaufman, J. J. See Chapman, D. A., 541
Kaur, S.
—; Ray, N. K.: A Non-Local Pseudopotential in the FSGO Model: Study of Some Organometallic Systems, 115
Keegstra, P. B. See Chapman, D. A., 541
Keller, J. See Castro, M., 689
Khan, A. U.
The Discovery of the Chemical Evolution of Singlet Oxygen. Some Current Chemical, Photochemical, and Biological Applications, 251
Klasinc, L. See McGlynn, S. P., 399
Koizumi, M. See Tachibana, A., 561
Krechl, J. See Tapia, O., 767
Kumar, D. See McGlynn, S. P., 399
Kunz, A. B. See Seel, M., 149

Ladik, J. See Fleck, O., 839
Lathouwers, L. See Broeckhove, J., 523
Lee, S.-L.
—; Li, F.-Y.; Lin, F.: Topological Analysis of Eigenvalues of Particle in One- and Two-Dimensional Simple Quantal Systems: Net Sign Approach, 59
Leonard, J. M. See Jensen, J. O., 163
Li, F.-Y. See Lee, S.-L., 59
Li, J. See Feng, J., 331
Li, Z. See Feng, J., 331
Lim, E. C. See Sobolewski, A. L., 309
Lin, F. See Lee, S.-L., 59
Lin, S. H. See Yeh, C. Y., 353
Linder, B.
Van der Waals Modulated Spectral Intensities: Application to Infrared Absorption, 437
Löwdin, P.-O.
International Journal of Quantum Chemistry—A Journal Devoted to Quantum Theory and Computations in Chemistry, Condensed Matter Physics, and Biology: Editorial—Program and Policies, 1

Some Current Problems in Quantum Chemistry as Described by Their Key Words and the International Journal of Quantum Chemistry, 3
Introduction to Issue in Honor of Michael Kasha, 231
Biographical Sketch of Michael Kasha, 235

Ma, H. See Yeh, C. Y., 353
Mann, A.
—; Green, A.: The Fate of the Dry Electron—A Preliminary Investigation, 47
March, N. H.
—; Santamaria, R.: Non-Local Relation Between Kinetic and Exchange Energy Densities in Hartree–Fock Theory, 585
—; See Nagy, A.: The Exact Form of the Pauli Potential for the Ground State of Two- and Three-Level Atoms and Ions, 615
Mareca, P. See Castro, M., 689
Massey, S. T.
—; Zoellner, R. W.: MNDO Calculations on Borazine Derivatives. The Substitution of One [HNBH] Fragment for One [HCCH] Fragment in Benzene to Form the Azaborines and the Nature of the Cyclotrimer of the 1,2-Isomer, 787
Matsuoka, O.
—; Fujimura, N.; Hasegawa, T.: Hydrogenlike Atoms in Uniformly Charged Sphere Model of Atomic Nucleus. II. Application of Basis-set Expansion Method, 813
—; See Hasegawa, T., 805
McGlynn, S. P.
—; Asaf, U.; Kumar, D.; Felps, S.; Rupnik, K.; Klasinc, L.: Solvent Effects in Dense Gases, 399
Mohamed, A. A. See Abu-Eittah, R., 211
Mohanty, A.
—; Clementi, E.: Dirac–Fock Self-Consistent Field Method for Closed-Shell Molecules with Kinetic Balance and Finite Nuclear Size, 487
Montagnani, R.
—; Tomasi, J.: The Influence of the Solvent on the Conformational Energy Differences Due to the Anomeric Effect, 851
Morrison, R. C.
—; Parr, R. G.: Approximate Density Matrices and Husimi Functions Using the Maximum Entropy Formulation with Constraints, 823
Muguet, F. F.
—; Robinson, G. W.; Bassez-Muguet, M.-P.: The Intermolecular Vibrations of the Bifurcated Water Dimer: An Ab Initio Study, 449
Murakhtanov, V. V. See Osadchii, M. S., 173
Murashima, M. See Tachibana, A., 561
Murrell, J. N.
—; Eriksson, L. A.; Bosanac, S. D.: A Comment on Classical Rainbow Angles for Atom-Atom Scattering, 159

Nagy, A.
—; March N. H.: The Exact Form of the Pauli Potential for the Ground State of Two- and Three-Level Atoms and Ions, 615
Nakatsuji, H.
—; Saito, S.: Excited and Ionized States of RuO_4 and OsO_4 Studied by SAC and SAC-CI Theories, 93

Oddershede, J.
—; Sabin, J. R.: Polarization Propagator Calculation of Spectroscopic Properties of Molecules, 371
—; See Sauer, S. P. A., 667
—; See Diercksen, G. H. F., 755
Olcina, V. Botella See Pacios, L. Fernandez, 197
Osadchii, M. S.
—; Murakhtanov, V. V.: The System of Harmonically Interacting Particles: An Exact Solution of the Quantum-Mechanical Problem, 173
Ovchinnikov, A. A. See Kariev, A. M., 131
Ozkabak, A. G.
—; Thakur, S. N.; Goodman, L.: Ab Initio Simulation of Benzene Raman Intensities, 411

Pacios, L. Fernandez
—; Olcina, V. Botella: A Correction to Effective Core Potentials for Transition Metals, 197
Paidarova, I. See Diercksen, G. H. F., 755
Parker, W. L.
—; Crosby, G. A.: Charge-Transfer Intensity in Complexes with Symmetrically Equivalent Acceptors, 299
Parr, R. G. See Morrison, R. C., 823
Parsons, I. W. See Howard, S. T., 71

Ramsay, D. A. See Fink, E. H., 287
Ray, N. K. See Kaur, S., 115
Rice, S. A. See Tersigni, S. H., 325
Robinson, G. W. See Muguet, F. F., 449
Roszak, S. See Chapman, D. A., 541
Rupnik, K. See McGlynn, S. P., 399

Sabin, J. R. See Oddershede, J., 371
—; Diercksen, G. H. F., 755
Saito, S. See Nakatsuji, H., 93
Santamaria, R. See March, N. H., 585
Sauer, S. P. A.
—; Diercksen, G. H. F.: Second-Order Polarization Propagator Calculations of Dynamic Dipole Polarizabilities and C_6 Coefficients, 667
Seel, M.
—; Kunz, A. B.: Band Structure and Electronic Properties of Lithium Azide (LiN_3), 149
Setzer, K. D. See Fink, E. H., 287
Shatkovskaya, D. See Gineitytė, 11
Shouping, J. See Jiancheng, X., 123
Siebrand, W. See Sobolewski, A. L., 309
Sobolewski, A. L.
—; Lim, E. C.; Siebrand, W.: Model Study of the Abrupt Excess-Energy Dependence of Radiationless Decay in Benzene and Azabenzenes, 309
Stanton, J. F.
Point Group Symmetry and Cartesian Force Constant Redundancy, 19
Steinborn, E. O. See Homeier, H. H. H., 625
Strickler, S. J.
—; Cormier, R. A.; Connolly, J. S.: Exciton Interactions in the Spectrum of a Dinaphthonorbornadiene, 345
Sun, H. See Kanzler, A. W., 269
Sutcliffe, B. T.
—; Tennyson, J.: A General Treatment of Vibration-Rotation Coordinates for Triatomic Molecules, 183

Tachibana, A.
—; Fueno, H.; Tanaka, E.; Murashima, M.; Koizumi, M.; Yamabe, T.: String Model for the Rate Constant of Nonadiabatic Solvation in the Hydration Reaction of Carbon Dioxide, 561
Tanaka, E. See Tachibana, A., 561
Tapia, O.
—; Cardenas, R.; Andres, J.; Krechl, J.; Campillo, M.; Colonna-Cesari, F.: Electronic Aspects of LADH Catalytic Mechanism, 767
Taylor, P. R.
Review of *Quantum Chemistry: Basic Aspects, Actual Trends*, edited by Ramon Carbó, 227
Tennyson, J. See Sutcliffe, B. T., 183
Tersigni, S. H.
—; Rice, S. A.: A Generalization of the Method of Stimulated Emission Pumping, 325
Thakur, S. N. See Ozkabak, A. G., 411
Thiel, Y.
—; Walters, V. A.; Wiberg, K. B.; Colson, S. D.: High-Resolution Infrared Analysis of the ν_{17} Band of Pyridine, 423
Till, S. J. See Howard, S. T., 71
Tomasi, J. See Montagnani, R., 851

Vervloet, M. See Fink, E. H., 287

Walters, V. A. See Thiel, Y., 423
Wasilewski, J.
Modified Virtual Orbitals (MVO) in Limited CI Calculations, 649
Wiberg, K. B. See Thiel, Y., 423
Wildt, J. See Fink, E. H., 287

Yamabe, T. See Tachibana, A., 561
Yeh, C. Y.
—; Chang, W. L.; Ma, H.; Lin, S. H.: Theory of Ultrafast Time-resolved Absorption Spectroscopy, 353

Zerner, M. C.
—; Anderson, W. P., 31
—; Feng, J., 331
Zhan, C.-G.
—; Zheng, F.: Maximum Overlap Symmetry Orbitals, 729
Zheng, F. See Zhan, C.-G., 729
Zoellner, R. W. See Massey, S. T., 787